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Filtered Density Function for Subgrid Scale Modeling of Turbulent Combustion

P. Givi and M.R.H. Sheikhi

Department of Mechanical Engineering and Materials Science
University of Pittsburgh
Pittsburgh, PA 15261

Abstract

This research was concentrated primarily on developments and applications of the filtered density function (FDF) for subgrid scale (SGS) modeling of turbulent reacting flows. During the past three years, this work addressed: (1) development of the joint velocity-scalar filtered mass density function (VSFMDF), (2) development of the joint frequency-velocity-scalar filtered mass density function (FVS-FMDF), and (3) implementation of the scalar filtered mass density function (SFMDF) and VSFMDF for large eddy simulation of complex turbulent flames. This is a final report of our activities sponsored by AFOSR under Grant FA9550-06-1-0015.

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1 Introduction

One the most challenging issues in combustion simulations is associated with turbulence, including turbulence-chemistry interactions. The phenomenon of mixing at both micro- and macro-scales and its role and capability (or lack thereof) to provide a suitable environment for combustion and the subsequent effects of combustion on hydrodynamics have been at the heart of turbulent combustion research for half a century now!

It is believed widely that the optimal means of capturing the detailed, unsteady physics of turbulent combustion is via large eddy simulation (LES) [1–6]. The primary challenge in such LES is accurate modeling of the subgrid scale (SGS) quantities [3]. The *Filtered Density Function* (FDF) methodology, including its mass weighted form, the *Filtered Mass Density Function* (FMDF) has proven particularly effective for this purpose [1, 7]. The FDF is essentially the counterpart of the *Probability Density Function* (PDF) method in Reynolds averaged simulation, commonly referred to as the Reynolds-averaged Navier-Stokes (RANS) [1]. The idea of using the PDF method for LES was suggested first by Givi [8], and the formal definition of FDF by Pope [9] provided the mathematical foundation of LES/FDF. In its simplest form, the “assumed” FDF method was suggested by Madnia *et al.* [10, 11], where all of the drawbacks of this *ad hoc* approach were highlighted. The “transported” (not-assumed) marginal scalar FDF (SFDF) was developed by Gao and O’Brien [12] and Colucci *et al.* [13]; the latter demonstrated that solution of the FDF from its own transport equation is possible. The scalar filtered mass density function (SFMDf), which is the variable density form of SFDF, was developed by Jaberri *et al.* [14, 15] and Garrick *et al.* [16]. The marginal velocity FDF (VFDF) was developed by Gicquel *et al.* [17]. The joint velocity-scalar FDF (VSFDF) was developed by Sheikhi *et al.* [18]. The first LES of a hydrocarbon flame, namely the Sandia-Darmstadt piloted diffusion flame [19, 20], was conducted via SFMDf [21].

The work of Colucci *et al.* [13] provides the first demonstration of a “transported” FDF. Since then, this methodology has experienced widespread usage and now is regarded as one of the most effective and popular means of LES worldwide. Some examples of recent contributions in FDF by others are in its basic implementation [22–36], fine-tuning of its sub-closures [37–39], and its validation via laboratory experiments [26, 40–44]. The FDF is finding its way into industry and commercial codes (Fluent/ANSYS) and has been the subject of detailed discussions in several text- and hand-books [1, 4, 5, 45–47]. Givi *et al.* [48] provide a recent review of the state of progress in LES via FDF.

2 Accomplishments

The goal of this research was to improve the capabilities of the FDF method and to implement it for LES of chemically reacting turbulent flows. We feel that we have

been very successful in achieving the specific objectives of this work. For a complete review of our work and our progress, we refer to the following publications:

- Development of VSFMDF. This work is published in Ref. [49].
- Application of SFMDF for LES of Sandia-Sydney Bluff-Body Flame. This work is published in Ref. [50].
- Development of FVS-FMDF. This work is submitted for publication [51].
- Application of VSFMDF for LES of Sandia-Darmstadt Piloted Jet Flame. This work is under progress [52].
- Several other papers are published including a survey [7], a tutorial [53], and two reviews [48,54]; including one in a Russian journal

3 Interaction with AFRL

We are very grateful to have the opportunity of interacting with several of the researchers at the Wright-Patterson AFB on several occasions. During the past three years we have had face-to-face meetings with several of the AFRL/VA and AFRL/PA scientists.

4 Publications

All of the publications resulting from this work within the past three years are listed here. AFOSR is acknowledged in all of these. Invited publications are identified by a ★

4.1 Review, Survey and Tutorials

★ M.R.H. Sheikhi, T.G. Drozda, C.K. Madnia, and P. Givi, "PDF Methods for LES of Turbulent Reactive Flows," Chapter in *Nonequilibrium Processes: Plasma, Combustion and Atmospheric Phenomena*, Editors: G.D. Roy, S.M. Frolov and A.M. Starik, in press (2009).

★ P. Givi, M.R.H. Sheikhi, T.G. Drozda and C.K. Madnia, "Invited Review: Reliable and Affordable Simulation of Turbulent Reacting Flows," AIAA Paper *AIAA-2007-0190* (2007).

★ C.K. Madnia, F.A. Jaber and P. Givi "Large Eddy Simulation of Heat and Mass Transport in Turbulent Flows," Chapter 5 in *Handbook of Numerical Heat Transfer*,

pp. 167–189, Second Edition, Editor: W.J. Minkowycz, E.M. Sparrow, and J.Y. Murthy, John Wiley & Sons, Inc., New York, NY (2006).

★ P. Givi, “Invited Survey: Filtered Density Function for Subgrid Scale Modeling of Turbulent Combustion,” *AIAA Journal*, **44**(1), 16–23 (2006).

4.2 Journal Articles

M.B. Nik, M.R.H. Sheikhi, P. Givi and S.B. Pope, “VSFMDf for Large Eddy Simulation of a Piloted Jet Flame,” to be submitted to *AIAA Journal* (2009).

★ P. Givi, M.R.H. Sheikhi, T.G. Drozda and C.K. Madnia, ”Large Scale Simulation of Turbulent Combustion,” *Combustion and Plasma Chemistry*(Russian), **6**(1), 1-6 (2008).

M.R.H. Sheikhi, P. Givi and S.B. Pope, “Joint Velocity-Scalar Filtered Mass Density Function for Large Eddy Simulation of Turbulent Reacting Flows,” *Physics of Fluids*, **19**(9), 095106 1-21 (2007).

★ T.G. Drozda, M.R.H. Sheikhi, C.K. Madnia and P. Givi, “Developments in Formulation and Application of the Filtered Density Function,” *Flow, Turbulence and Combustion*, **78**, 35-67 (2007).

4.3 Conference Papers

★ P. Givi and M.R.H. Sheikhi, “FDF Methods in Turbulent Combustion,” Proceedings of the International Symposium on Recent Advances in Combustion and Noise Control for Propulsion, p. 7, Kauai, HI, December 10-12, 2008.

M.R.H. Sheikhi, P. Givi and S.B. Pope, “Implementation of the Joint Frequency-Velocity-Scalar Filtered Mass Density Function for Large Eddy Simulation of Turbulent Reacting Flows,” *Bulletin of the American Physical Society*, **53**(15), p. 60, 61st Annual Meeting of the Division of Fluid Dynamics of the American Physical Society, San Antonio, TX, November 23-25, 2008.

★ T.G. Drozda, M.R.H. Sheikhi, C.K. Madnia and P. Givi, “Structure of Turbulent Diffusion Flames,” Proceedings of the International Conference in Computational and Informational Technologies in Science, Engineering and Education, Almaty, Kazakhstan, September 10-14, 2008.

★ M.R.H. Sheikhi, T.G. Drozda, C.K. Madnia and P. Givi, “Structure of Nonpremixed Turbulent Flames,” Proceedings of the 7th International Symposium on Hazards, Prevention and Mitigation of Industrial Explosions, pp. 141-154, St. Petersburg, Russia, July 7-11, 2008.

★ P. Givi, "The Impact of ONR-YIP: An Example," Proceedings of ONR 20th 20th Propulsion Meeting, pp. 1-8, Arlington, VA, December 12-14, 2007.

M.B. Nik, M.R.H. Sheikhi, P. Givi and S.B. Pope, "VSFMDF for LES of Sandia's Turbulent Piloted Jet Flame," *Bulletin of the American Physical Society*, **52**(17), pp. 217-218, 60th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society, Salt Lake City, UT, November 18-20, 2007.

P. Givi, M.R.H. Sheikhi and S.B. Pope, "Development of Joint Frequency-Velocity-Scalar Filtered Mass Density Function for Large Eddy Simulation of Turbulent Reacting Flows," Proceedings of the 4th International Symposium on Combustion and Plasma Chemistry, pp. 18-20, Almaty, Kazakhstan, September 12-14, 2007.

M.R.H. Sheikhi, P. Givi and S.B. Pope, "Joint Frequency-Velocity-Scalar Filtered Mass Density Function for Large Eddy Simulation of Turbulent Reacting Flows," *Bulletin of the American Physical Society*, **51**(9), p. 127, 59th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society, Tampa Bay, FL, November 19-21, 2006.

★ P. Givi, "A Novel Strategy for Turbulent Combustion Simulation," Keynote Presentation IMECE2006-16563, ASME International Mechanical Engineering Congress and Exhibition, Chicago, Illinois, November 5-10, 2006.

★ P. Givi, "Large Eddy Simulation of Turbulent Combustion," Proceedings of the Second International Scientific Conference on Problems of Modern Mechanics, pp. 26-33, Almaty, Kazakhstan, September 7-8, 2006.

P. Givi, M.R.H. Sheikhi and S.B. Pope, "Latest Developments in Formulation and Application of the Filtered Density Function," SIAM Conference on Numerical Combustion, April 23-26, 2006, Granada, Spain.

4.4 Awards and Honors

During the past three years, the PI of this Grant received the following awards:

1. P. Givi named Engineer of the Year Award by ASME, Pittsburgh Section (2007).
2. P. Givi was named Fellow of American Physical Society (2007). Citation: "For Pioneering Computational Research on Turbulent Reactive Flows, and Especially for the Development of the Filtered Density Function Methodology."
3. P. Givi was elected Fellow of American Society of Mechanical Engineers (2006).

5 Public Lectures

During the course of this research, the PI delivered the following invited lectures and seminars with acknowledgement of AFOSR. All of the invited presentations are identified by a *.

5.1 Invited Keynote & Plenary Lectures at Conferences

- * "Structure of Nonpremixed Turbulent Flames," 7th International Symposium on Hazards, Prevention and Mitigation of Industrial Explosions, St. Petersburg, Russia, July 8, 2008.
- * "The Impact of ONR-YIP: An Example," 20th ONR Propulsion Meeting, Arlington, VA, December 12, 2007.
- * "PDF Methods for LES of Turbulent Reactive Flows," Third International Symposium on Nonequilibrium Processes, Plasma, Combustion and Atmospheric Phenomena, Sochi, Russia, June 25, 2007.
- * "Reliable and Affordable Simulation of Turbulent Reacting Flows," Paper *AIAA-2007-0190*, 45th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, January 8, 2007.
- * "A Novel Strategy for Turbulent Combustion Simulation," ASME International Mechanical Engineering Congress and Exhibition, Chicago, Illinois, November 7, 2006
- * "Large Eddy Simulation of Turbulent Combustion," Second International Scientific Conference on Problems of Modern Mechanics, Almaty, Kazakhstan, September 8, 2006.

5.2 Invited Seminars and Lectures

- * "Large Eddy Simulation of Turbulent Combustion," Department of Mechanical Science and Engineering, **University of Illinois at Urbana-Champaign**, Urbana, IL, November 7, 2008.
- * "Large Eddy Simulation of Turbulent Combustion," Department of Mechanical and Industrial Engineering, **Northeastern University**, Boston, MA, May 13, 2008.
- * "Large Eddy Simulation of Turbulent Combustion," Computer and Computational Sciences, **Los Alamos National Laboratory**, Los Alamos, NM, May 8, 2008.
- * "Large Scale Computation and Mathematical Modeling of Turbulent Combustion

and Propulsion,” Department of Mechanical Engineering, **Carnegie Mellon University**, Pittsburgh, PA, March 28, 2008.

★ “Latest Development in PDF Methods,” **Simulent Inc.**, Toronto, ON, Canada, March 21, 2008.

★ “A Novel CFD Methodology,” Department of Mechanical Engineering, **Iowa State University**, Ames, IA, October 2, 2007.

★ “Some Current Challenges in Computational Physics,” Institute of Mathematics, **Kazakhstan Academy of Science and Education**, Republic of Kazakhstan, Almaty, Kazakhstan, September 21, 2007.

★ “A Novel CFD Methodology,” Department of Mechanical and Aerospace Engineering, **University of Miami**, Coral Gables, FL, August 15, 2007.

★ “A Novel CFD Methodology,” **Simulent Inc.**, Toronto, ON, Canada, August 3, 2007.

★ “A Novel CFD Methodology,” College of Marine Sciences, **University of South Florida**, St. Petersburg, FL, April 23, 2007.

★ “The FDF vs. the PDF,” Institute of Problems of Burning,” El-Faraby **Kazak National University**, Almaty, Kazakhstan, September 14, 2006.

★ “A Novel Lagrangian-Eulerian Algorithm for Solving Multidimensional Hyperbolic Equations,” **Simulent Inc.**, Toronto, ON, Canada, July 21, 2006.

★ “Affordable and Reliable Prediction of Turbulent Combustion,” School of Industrial Engineering, **University of Málaga**, Málaga, Spain, April 27, 2006.

★ “Affordable and Reliable Prediction of Turbulent Combustion,” Department of Mechanical and Aerospace Engineering, University of Texas at Arlington, Arlington, TX, April 7, 2006.

★ “Affordable and Reliable Prediction of Turbulent Combustion,” Department of Aerospace Engineering, **University of Texas at Austin**, Austin, TX, April 6, 2006.

★ “Affordable and Reliable Prediction of Turbulent Combustion,” Department of Mechanical Engineering, **University of Utah**, Salt Lake City, UT, February 3, 2006.

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